NISTTech

Apparatus And Methods For Identifying and Comparing Lattice Structures and Determining Lattice Structure Symmetries

Description

Uses a matrix approach to represent physical crystals in idealized mathematical lattices to speed up and reduce error in identifying, classifying, and understanding the physical properties of materials. The approach is based on group theory and linear algebra offering a more abstract and powerful way look at crystal lattices and their properties.

Applications

- **Crystallography**
  Assists in further analysis and identification of a crystalline structure under investigation to determine its symmetry characteristics.
- **Materials Design**
  Assists in identifying related compounds for evaluation of a desired trait, e.g., compounds related to a new superconducting material. Easily determines lattice relationships in two apparently different materials exhibiting the same property. Helps to identify an unknown phase by rapidly matching the unknown against all known lattice structures. Assists in analysis of structural lattice relationships within a large set of compounds, or between two sets of compounds.

Advantages

- **More Effective**
  Substantially more effective than prior approaches because it maintains its selectivity in matching lattice structures despite the rather large experimental errors that are routinely associated with electron diffraction data. Errors in strategy are impossible with the matrix approach because at each step exactly the right data for control decisions are directly available in a clear, logical and concise format. Uses a three dimensional technique similar to that employed in single crystal x-ray and neutron diffractometry. Able to determine the cell structure and symmetry from data collected on extremely small samples and to identify the structure using computerized databases of known structures.
- **Greater Simplicity**

Simplifies the determination of standard or conventional cells by working with symmetry directly in the form of matrices, and not with the magnitude of lattice parameters and their associated errors. Calculations are straightforward and a transformation matrix is found using linear algebra techniques. Does not require that the lattice and its symmetry be expressed with respect to a standard cell or a standard orientation. Enables computer-based controllers for commercial diffractometers (x-ray, neutron and electron) to be implemented which fully automate the diffractometry process in a theoretically and experimentally correct and error-free manner.

Abstract

A converse transformation matrix generation approach is used either i) to relate a lattice structure of one crystalline material to the lattice structure(s) of one or more other crystalline materials for determining interlattice relationships which allow materials to be identified and classified relative to other materials; or ii) to relate a lattice structure of a material to itself for determining lattice symmetry. In particular, matrices which transform any primitive cell defining a lattice structure either into itself or into another cell defining a second lattice structure to within predetermined maximum tolerances of the cell parameters are generated.

Inventors

- Karen, Vicky L.
- Migdall, Alan

Citations

1. See expired Parent U.S. Patent # 5,168,457 Apparatus for identifying and comparing lattice structures and determining lattice structure symmetries
2. A. Mighell. Lattice symmetry and identification -the fundamental role of reduced cells in materials characterization. J. Res. Natl. Inst. Stand. Technol. 106, 983–995 (2001).
3. V. L. Himes and A. D. Mighell. A Matrix approach to symmetry. Acta Cryst. A43, 375-384 (19987).

References

- U.S. Patent # 5,235,523
- Docket: 92-042D

Status of Availability

This invention is available for licensing.

Last Modified: 09/03/2009